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Numerical solution of the inverse spectral problem for Bessel operators

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ABSTRACT

We consider some inverse spectral problems associated with the singular Sturm–Liouville equation

$$-u'' + \left(q(x) + \frac{\ell(\ell+1)}{x^2}\right)u = \lambda u \quad 0 < x < 1$$

for $\ell = 1, 2 \ldots$, which is obtained by separation of variables in the 3D radial Schrödinger equation. One approach to such problems involves the use of almost isospectral transformations, by means of which a reduction to a similar problem in the classical $\ell = 0$ case is possible. In this paper we focus on the development of computational techniques suggested by these ideas.

1. Problem statement

Let $q \in L^2(0, 1)$ be real valued, ℓ be a nonnegative integer, and define the Bessel operator

$$Lu = -u'' + \left(q(x) + \frac{\ell(\ell+1)}{x^2}\right)u \tag{1.1}$$

which is obtained, for example, after separation of variables for an elliptic operator with radially symmetric potential in the unit ball of $\mathbb{R}^3$. In this article we are interested in some aspects of inverse spectral theory for L in the singular case when $\ell > 0$, which are mainly related to issues of numerical solution in the case of the Dirichlet spectrum. Theoretical study of various versions of the singular inverse Sturm–Liouville problem can be found in a number of papers which are for the most part relatively recent in comparison to the large literature for the regular ($\ell = 0$) case—specific references will be given below. To the best of our knowledge there are very few works specifically concerned with computational methods in the singular case—see [1] for one recent paper.

Keeping in mind that a number of effective numerical solution methods have been developed for regular inverse spectral problems there are two approaches that one might take for the singular case. One is to simply adapt one of the known methods for $\ell = 0$ to handle the singularity in the equation. A second, slightly less obvious approach, is to seek some way to transform the singular problem to some corresponding regular problem, and then take advantage of one of the well developed methods for that case. Techniques first appearing in [2] and elaborated recently in [3] indicate one precise way to do this. Deriving and illustrating a constructive numerical algorithm based on these ideas will be the main focus of this paper. Attention will mainly be paid to the two representative cases $\ell = 1$ and $\ell = 2$. We might mention that in the context of p-wave inverse scattering for a central potential, the possibility to transform from a singular case to the regular case appears in the work of Marchenko (see [4], p. 70), and could be the basis for an effective numerical method in that situation also.

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1.1. Eigenvalues and norming constants

We will assume that the given spectral data is of the eigenvalue/norming constant type corresponding to a Dirichlet boundary condition at $x = 1$ in the singular ($\ell > 0$) case. There are several different definitions of norming constant which seem natural, and we begin by clarifying their properties and relationships to each other.

It is well known (see e.g. [5] for some detailed estimates) that for any $\lambda \in \mathbb{C}$ there exists a unique regular function $\phi(\cdot, \lambda)$ which is the solution of

$$L\phi = \lambda\phi \qquad \lim_{x\to 0+} (2\ell + 1)!!x^{-\ell-1}\phi(x, \lambda) = 1. \tag{1.2}$$

Any solution to $Lu = \lambda u$ that is linearly independent of ϕ is $O(x^{-\ell})$ at the origin, so that the differential expression is in the limit circle case at $x = 0$ for $\ell = 0$ and in the limit point case there if $\ell > 0$. Therefore realizations of L do not need any boundary condition at the point $x = 0$ in the latter case; in particular, it is known that the operator L subject to the Dirichlet boundary condition $u(1) = 0$ is self-adjoint in $L^2(0, 1)$ and has a discrete spectrum. The corresponding eigenvalues are those λ for which there exists $u \not\equiv 0$ satisfying

$$Lu = \lambda u \qquad |u(0)| < \infty \qquad u(1) = 0. \tag{1.3}$$

They coincide with solutions of $\phi(1, \lambda) = 0$ and may be given as an increasing sequence $\{\lambda_n\}_{n=1}^{\infty}$ satisfying (see e.g. [5])

$$\lambda_n = \left(\left(n + \frac{\ell}{2}\right)\pi\right)^2 + \int_0^1 q(x)\,\mathrm{d}x - \ell(\ell + 1) + a_n \qquad \sum_{n=1}^{\infty} a_n^2 < \infty. \tag{1.4}$$

For later use, let us define $\phi_0(x, \lambda)$ to be the special case of ϕ when $q \equiv 0$, namely

$$\phi_0(x, \lambda) = \frac{xj_\ell\left(\sqrt{\lambda}x\right)}{\lambda^{\frac{\ell}{2}}} \tag{1.5}$$

where j_ℓ is the usual spherical Bessel function. Denote by $\lambda_{0,n}$ the eigenvalues corresponding to $q(x) \equiv 0$, so that $\{\sqrt{\lambda_{0,n}}\}$ are the zeros of j_ℓ.

There are four sets of norming constants which might naturally be associated with the above eigenvalue problem, three of which have appeared previously in the literature. To define them, first introduce $\psi(\cdot, \lambda)$, the solution of the initial value problem

$$L\psi = \lambda\psi \qquad \psi(1, \lambda) = 0 \qquad \psi'(1, \lambda) = 1. \tag{1.6}$$

One has that ψ is regular on $(0, 1]$ with $\psi(x) = O(x^{-\ell})$ as $x \to 0$ unless $\lambda = \lambda_n$ is a Dirichlet eigenvalue, in which case $\phi_n := \phi(\cdot, \lambda_n)$ and $\psi_n = \psi(\cdot, \lambda_n)$ are linearly dependent eigenfunctions. We denote

$$\rho_n^+ = \int_0^1 \psi_n^2(x)\,\mathrm{d}x \tag{1.7}$$

$$\rho_n^- = \int_0^1 \phi_n^2(x)\,\mathrm{d}x \tag{1.8}$$

$$\gamma_n = \phi_n'(1) \tag{1.9}$$

$$k_n = \log\left[\frac{\phi_n'(1)}{\phi_0'(1, \lambda_{0,n})}\right]. \tag{1.10}$$

1.2. Statement of inverse spectral problems

We may consider the problem of recovering q from the eigenvalues λ_n and any one of the sets of norming constants. For definiteness we label these problems as

- Problem 1: ([2,3]) Find q given $\{\lambda_n, \rho_n^+\}_{n=1}^{\infty}$.
- Problem 2: Find q given $\{\lambda_n, \rho_n^-\}_{n=1}^{\infty}$.
- Problem 3: ([5,6]) Find q given $\{\lambda_n, \gamma_n\}_{n=1}^{\infty}$.
- Problem 4: ([7,8]) Find q given $\{\lambda_n, k_n\}_{n=1}^{\infty}$.

We next observe that the four problems are equivalent to each other. Obviously the difference between Problems 3 and 4 is a trivial one—the purpose of introducing the $\phi_0(1, \lambda_{0,n})$ factor is normalization, to achieve that $\{k_n\}$ belongs to a convenient sequence space.

1.3. Relationships between norming constants

Evidently we have

$$\gamma_n^2 = \left[\frac{\phi_n(x)}{\psi_n(x)}\right]^2 = \frac{\rho_n^-}{\rho_n^+} \tag{1.11}$$

and as already noted, knowledge of γ_n and k_n are equivalent. In fact we have

$$\phi_0'(1, \lambda_{0,n}) = \lambda_{0,n}^{\frac{1-\ell}{2}} j_\ell' \left(\sqrt{\lambda_{0,n}}\right) \tag{1.12}$$

where $\lambda_{0,n}$ is in principle known.

Next we establish a relationship between ρ_n^+ and γ_n. Define the Wronskian

$$W = \phi(x,\lambda)\psi'(x,\lambda) - \phi'(x,\lambda)\psi(x,\lambda). \tag{1.13}$$

It is independent of $x \in (0, 1]$ and so

$$W = W(\lambda) = \phi(1,\lambda). \tag{1.14}$$

W is thus an entire function with real roots $\{\lambda_n\}_{n=1}^\infty$ which make up the spectrum of the singular Sturm–Liouville problem (1.3).

Lemma 1.1. *For every n we have*[1]

$$\gamma_n \rho_n^+ = -\frac{j_\ell\left(\sqrt{\lambda_n}\right)}{\lambda_n^{\frac{\ell}{2}}(\lambda_{0,n} - \lambda_n)} \prod_{m \neq n} \frac{\lambda_m - \lambda_n}{\lambda_{0,m} - \lambda_n}. \tag{1.15}$$

Proof. Assume that λ is not an eigenvalue, and consider the solution $u = u(x,\lambda)$ of

$$\lambda u - Lu = f \quad 0 < x < 1 \qquad |u(0)| < \infty \quad u(1) = 0. \tag{1.16}$$

By standard completeness results we can express u as an eigenfunction expansion

$$u(x,\lambda) = \sum_{n=1}^\infty \frac{(f, \psi_n)\psi_n(x)}{\rho_n^+(\lambda - \lambda_n)}. \tag{1.17}$$

On the other hand, we may also express u by means of the variation of parameters formula

$$u(x,\lambda) = \frac{\psi(x,\lambda)}{W(\lambda)} \int_0^x \phi(s,\lambda) f(s)\, ds + \frac{\phi(x,\lambda)}{W(\lambda)} \int_x^1 \psi(s,\lambda) f(s)\, ds. \tag{1.18}$$

Here we are using the asymptotics of ϕ and ψ as $x \to 0$ in order to verify that $u(0,\lambda)$ is finite.

Now the residue expression $R_n(x) = \lim_{\lambda \to \lambda_n} (\lambda - \lambda_n) u(x,\lambda)$ satisfies

$$R_n = \frac{(f, \psi_n)\psi_n(x)}{\rho_n^+} \tag{1.19}$$

and

$$R_n = \frac{\psi(x,\lambda_n)}{\dot W(\lambda_n)} \int_0^x \phi(s,\lambda_n) f(s)\, ds + \frac{\phi(x,\lambda_n)}{\dot W(\lambda_n)} \int_x^1 \psi(s,\lambda_n) f(s)\, ds. \tag{1.20}$$

Using $\phi(x,\lambda_n) = \phi_n(x) = \gamma_n \psi_n(x)$, $\psi(x,\lambda_n) = \psi_n(x)$ this implies

$$\frac{(f, \psi_n)\psi_n(x)}{\rho_n^+} = \frac{\gamma_n (f, \psi_n)\psi_n(x)}{\dot W(\lambda_n)} \tag{1.21}$$

i.e.

$$\frac{\partial \phi}{\partial \lambda}(1, \lambda_n) = \dot W(\lambda_n) = \gamma_n \rho_n^+. \tag{1.22}$$

[1] In case $\lambda_n = \lambda_{0,k}$ for some $k \in \mathbb{N}$, we must replace the fraction $\frac{j_\ell(\sqrt{\lambda_n})}{\lambda_{0,k} - \lambda_n}$ with the limiting expression $-\frac{j_\ell'(\sqrt{\lambda_{0,k}})}{2\sqrt{\lambda_{0,k}}}$.

Now we know that $\phi(1,\lambda)$ is uniquely determined by its zeros, which are precisely the eigenvalues $\{\lambda_n\}$. In fact by a fairly standard argument (see Lemma 1.2 below) we can show that

$$\phi(1,\lambda) = \frac{1}{(2\ell+1)!!}\prod_{m=1}^{\infty}\frac{\lambda_m-\lambda}{\lambda_{0,m}}. \tag{1.23}$$

It follows that

$$\frac{\partial\phi}{\partial\lambda}(1,\lambda_n) = -\frac{\phi_0(1,\lambda_n)}{\lambda_{0,n}-\lambda_n}\prod_{m\neq n}\frac{\lambda_m-\lambda_n}{\lambda_{0,m}-\lambda_n} \tag{1.24}$$

where we use that

$$\phi_0(1,\lambda) = \frac{1}{(2\ell+1)!!}\prod_{m=1}^{\infty}\left(1-\frac{\lambda}{\lambda_{0,m}}\right) \tag{1.25}$$

and the conclusion then follows from (1.5). $\square$

From (1.11), (1.12) and Lemma 1.1 it follows that given the eigenvalues $\{\lambda_n\}$, knowledge of any one of the sets of norming constants is equivalent to knowledge of any other set.

Lemma 1.2. *The identity (1.23) holds.*

Proof. Since $\phi(1,\lambda)$ is an entire function of exponential type 1/2, the Hadamard factorization gives

$$\phi(1,\lambda) = C\prod_{n=1}^{\infty}\left(1-\frac{\lambda}{\lambda_n}\right) \tag{1.26}$$

for some constant C. If C_0 denotes the corresponding constant for $q=0$ we get

$$\frac{\phi(1,\lambda)}{\phi_0(1,\lambda)} = \frac{C}{C_0}\prod_{n=1}^{\infty}\frac{\lambda_n-\lambda}{\lambda_{0,n}-\lambda}\prod_{n=1}^{\infty}\frac{\lambda_{0,n}}{\lambda_n}. \tag{1.27}$$

Taking the limit as $\lambda\to-\infty$ and using known asymptotics (see [5], Lemma 3.2) we get $\phi(1,\lambda)/\phi_0(1,\lambda)\to 1$ and consequently

$$C = C_0\prod_{n=1}^{\infty}\frac{\lambda_n}{\lambda_{0,n}}. \tag{1.28}$$

Since by direct calculation we see that $C_0=\phi_0(1,0)=1/(2\ell+1)!!$, the conclusion follows. $\square$

1.4. Asymptotics of the norming constants

Using some known estimates on the behavior of ρ_n^+ and k_n as $n\to\infty$ and the above relationships, we can make some conclusions about the asymptotic behavior in all cases. We write $a_n\approx b_n$ if $a_n=b_n(1+o(1))$ as $n\to\infty$.

Proposition 1.3. *The norming constants have the asymptotic behaviors*

$$\rho_n^+ \approx \frac{1}{2(n\pi)^2} \tag{1.29}$$

$$\rho_n^- \approx \frac{1}{2(n\pi)^{\ell+2}} \tag{1.30}$$

$$\gamma_n \approx \frac{(-1)^n}{(n\pi)^{\frac{\ell}{2}}} \tag{1.31}$$

$$k_n = o\left(\frac{1}{n}\right). \tag{1.32}$$

Remark. The proof will contain some slightly more refined estimates.

Proof. Asymptotics for ρ_n^+ may be found from [3] (note that, in the formula (1.7) there, $g_2\in H^1(0,1)$),

$$\rho_n^+ = \frac{1}{\lambda_n\left(2+\frac{b_n}{n}\right)} \qquad \sum_{n=1}^{\infty}b_n^2<\infty \tag{1.33}$$

or using (1.4)

$$\rho_n^+ = \frac{1}{2\pi^2 n^2} - \frac{\ell}{2\pi^2 n^3} + o\left(\frac{1}{n^3}\right). \tag{1.34}$$

If there exists the limit $\beta = \lim_{n\to\infty} nb_n$, as will be the case for smooth enough q, then the expansion may be continued as

$$\rho_n^+ = \frac{1}{2\pi^2 n^2} - \frac{\ell}{2\pi^2 n^3} + \frac{C_0}{n^4} + o\left(\frac{1}{n^4}\right) \tag{1.35}$$

where

$$C_0 = \frac{1}{2\pi^2}\left[\frac{3}{4}\ell^2 + \frac{\ell(\ell+1) - \int_0^1 q(x)\,dx}{\pi^2} - \frac{\beta}{2}\right]. \tag{1.36}$$

From [8] (or [7] in the case of $\ell = 1$) we have that

$$k_n = \frac{c_n}{n} \qquad \sum_{n=1}^{\infty} c_n^2 < \infty \tag{1.37}$$

from which it follows that

$$\gamma_n \approx \left(1 + \frac{c_n}{n}\right)\phi_0'\left(1, \sqrt{\lambda_{0,n}}\right). \tag{1.38}$$

From known asymptotic properties of Bessel functions and (1.4), we get

$$\phi_0'(1, \sqrt{\lambda_{0,n}}) \approx \frac{(-1)^n}{\left(\left(n+\frac{\ell}{2}\right)\pi\right)^{\frac{\ell}{2}}} \tag{1.39}$$

and it then follows that

$$\gamma_n \approx \frac{(-1)^n}{(n\pi)^{\frac{\ell}{2}}} \tag{1.40}$$

$$\rho_n^- \approx \frac{1}{2(n\pi)^{\ell+2}}. \quad \square \tag{1.41}$$

1.5. Previous work on the inverse spectral problem

The first study of Problem 1 in the singular case $\ell > 0$, or rather the analogous problem when the boundary condition at $x = 1$ is of Robin type, seems to occur in [2]. Sufficient conditions are given on sequences $\{\lambda_n\}$, $\{\rho_n^+\}$ for there to exist some $q \in L^2(0, 1)$ possessing these sequences as spectral data, but no specific claim about uniqueness is given. In [3] this work is generalized in several ways, including a more general class of q's, clear statements concerning uniqueness, and inclusion of the case when the Dirichlet boundary condition is prescribed at $x = 1$. In both works, an essential idea is the use of Darboux type transformation to relate the given singular inverse spectral problem to a corresponding problem with $\ell = 0$. This property distinguishes Problem 1 from the other three cases.

In [5] it is proved that uniqueness holds for Problem 3, as well as for analogous problems with other boundary conditions at $x = 1$ and for the case when norming constant data is replaced by a second spectrum, corresponding to a distinct boundary condition at $x = 1$. The constant ℓ there can be any real number greater than or equal to $-\frac{1}{2}$. In [6] a somewhat different approach modeled on [9] is used to prove the same uniqueness theorem for $q \in L^1(0, 1)$. Problem 4 is first studied in [7] for the case $\ell = 1$. The uniqueness result is stated, but the main interest there is in the analytic structure of the mapping from potential to spectral data and properties of the isospectral sets. Corresponding results for $\ell = 2, 3, \ldots$ are given in [8]. Finally, we know of no previous work explicitly on the case of Problem 2.

In any case we may state

Theorem 1.4. *A potential $q \in L^2(0, 1)$ is uniquely determined by any one of the data sets listed in Section 1.2.*

2. Constructive solution of Problem 1

Since all four inverse spectral problems are equivalent to each other in a rather straightforward way, we will focus on the use of the data $\{\lambda_n, \rho_n^+\}$, since as remarked earlier, the data in this case may be most directly related to a corresponding inverse problem for $\ell = 0$, where we can take best advantage of known techniques. It turns out that there is an essential difference between the case of ℓ odd and ℓ even. The latter is the simpler case, and to represent it we will focus on the case $\ell = 2$. After that we will turn to the case of $\ell = 1$.

2.1. The case $\ell = 2$

Let us recall (e.g. [10], Theorem 1.3 with $s = 1$)[2] that two sequences $\{\mu_n\}_{n=1}^{\infty}$ and $\{\sigma_n\}_{n=1}^{\infty}$ of real numbers are the eigenvalues and associated norming constants for the regular Dirichlet problem

$$-u'' + Q(x)u = \lambda u \quad 0 < x < 1 \qquad u(0) = u(1) = 0 \tag{2.1}$$

for some $Q \in L^2(0, 1)$, if and only if $\{\mu_n\}$ is a strictly increasing sequence having the representation

$$\mu_n = (n\pi)^2 + C_0 + \alpha_n \qquad \sum_{n=1}^{\infty} \alpha_n^2 < \infty \tag{2.2}$$

while $\{\sigma_n\}$ is a positive sequence having the form

$$\sigma_n = \frac{1}{2(n\pi)^2}\left(1 + \frac{\beta_n}{n}\right) \qquad \sum_{n=1}^{\infty} \beta_n^2 < \infty. \tag{2.3}$$

The norming constant definition we use here is

$$\sigma_n := \frac{\|u_n\|_{L^2}^2}{u_n'(1)^2} \tag{2.4}$$

where u_n is an eigenfunction for μ_n, i.e. it is exactly the definition of ρ_n^+ in the $\ell = 0$ case.

Now choose any value $\widehat{\lambda} < \lambda_1$ and let

$$\mu_n = \begin{cases} \widehat{\lambda} & n = 1 \\ \lambda_{n-1} & n \geq 2. \end{cases} \tag{2.5}$$

Then $\mu_n = (n\pi)^2 + C_0 + a_{n-1}$ with $C_0 = \int_0^1 q(s)\,\mathrm{d}s - 6$. From well known results about the $\ell = 0$ case (e.g. [9]), it follows that there exists $Q \in L^2(0, 1)$ with $\int_0^1 Q(s)\,\mathrm{d}s = C_0$ (in fact infinitely many such Q) for which the problem (2.1) has spectrum $\{\mu_n\}$. Likewise if we choose any value $\widehat{\rho}^+ > 0$ and let

$$\sigma_n = \begin{cases} \widehat{\rho}^+ & n = 1 \\ \rho_{n-1}^+ & n \geq 2 \end{cases} \tag{2.6}$$

then it is straightforward to check that (2.3) holds with some ℓ^2 sequence β_n depending on a_n, b_n and $\int_0^1 q(s)\,\mathrm{d}s$. There exists then a unique $Q \in L^2(0, 1)$ for which (2.1) has spectral data $\{\mu_n, \sigma_n\}$, and

$$\int_0^1 Q(s)\,\mathrm{d}s = \int_0^1 q(s)\,\mathrm{d}s - 6. \tag{2.7}$$

The key point now (see (C.13) with $\ell = 0$) is that q and Q are related by

$$q(x) = Q(x) - \frac{6}{x^2} - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\theta(x) \tag{2.8}$$

where

$$\theta(x) = \int_0^x \widehat{\psi}^2(s)\,\mathrm{d}s \tag{2.9}$$

and $\widehat{\psi}$ denotes the solution of

$$\psi'' + (\widehat{\lambda} - Q(x))\psi = 0 \qquad \psi(1) = 0 \qquad \psi'(1) = \frac{1}{\sqrt{\widehat{\rho}^+}}. \tag{2.10}$$

A similar result is formulated implicitly in [2], see also [11] for related properties in the context of inverse scattering.

Note that $\widehat{\psi}$ is an eigenfunction corresponding to the Dirichlet eigenvalue $\widehat{\lambda}$ for the potential Q and thus $\widehat{\psi}(x) = x\widehat{\eta}(x)$ for some $\widehat{\eta} \in H^2(0, 1)$, see Lemma B.3. It follows from Corollary B.2 that $\theta(x) = x^3\eta(x)$ for some $\eta \in H^2(0, 1)$ that is positive on $[0, 1]$, so that the combination $\frac{6}{x^2} + 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\theta(x) = 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\eta(x)$ gives a function in $L^2(0, 1)$.

The end result is that we can determine q in a constructive manner by first obtaining $Q(x)$, then successively using (2.10) to get $\widehat{\psi}$, (2.9) to get θ and finally (2.8) to obtain q. All of these steps are unambiguous, and may be implemented numerically, see Section 3. Clearly Q depends on the choices of $\widehat{\lambda}$ and $\widehat{\rho}^+$ which are made, but the uniqueness results discussed earlier guarantee that we obtain the correct q in any case. Note also that the singularity of the potential plays no role at all until the final step.

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[2] We believe that this special case was known well before [10] but could not find an explicit reference. See [9] for the corresponding necessary and sufficient conditions when the norming constants are defined in one of the alternate ways.

Example. As an analytical example of the procedure just outlined, we can compute the solution of the inverse spectral problem for the case that

$$\lambda_n = ((n+1)\pi)^2 \qquad \rho_n^+ = \frac{1}{2((n+1)\pi)^2}. \tag{2.11}$$

Choose $\widehat{\lambda} = \pi^2,\ \widehat{\rho}^+ = \frac{1}{2\pi^2}$. We then have $Q \equiv 0$ from which we may compute that

$$\widehat{\psi}(x) = -\sqrt{2}\sin \pi x \qquad \theta(x) = x - \frac{\sin 2\pi x}{2\pi} \tag{2.12}$$

and finally

$$q(x) = \frac{16\pi^2(1-\cos 2\pi x - \pi x \sin 2\pi x)}{(2\pi x - \sin 2\pi x)^2} - \frac{6}{x^2} \tag{2.13}$$

which may be verified to belong to $L^2(0, 1)$.

2.2. Alternative approach

In the previous section, the map $Q \to q$ amounts to an eigenvalue removal transformation, that is, all eigenvalues and norming constants of q are the same as those for Q, except that the first pair is dropped. There is an analogous eigenvalue addition procedure, corresponding to the inverse map $q \to Q$ which could also be exploited.

Suppose that $\widehat{\lambda} < \lambda_1$ and $\widehat{\rho}^+ > 0$ are any fixed constants, let $\widehat{\psi}(x)$ be the solution of

$$\psi'' + \left(\widehat{\lambda} - \frac{6}{x^2} - q(x)\right)\psi = 0 \qquad \psi(1) = 0 \qquad \psi'(1) = \frac{1}{\sqrt{\widehat{\rho}^+}} \tag{2.14}$$

and

$$\theta(x) = 1 + \int_x^1 \widehat{\psi}(s)^2\, \mathrm{d}s. \tag{2.15}$$

We may then define a mapping Γ by

$$\Gamma(q) = \frac{6}{x^2} - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\theta(x). \tag{2.16}$$

Some properties of Γ are given in Appendix B. It follows again that (see (C.14) with $\ell = 2$)

$$q + \Gamma(q) = Q \tag{2.17}$$

holds, where Q is defined as in the previous section to be the solution of the regular inverse spectral problem with the augmented data sets. The map $I + \Gamma$ in effect adds one prescribed eigenvalue and norming constant to the original spectral data, and so can be recognized as a particular case of the double commutation method, see [12].

By Lemma B.4, $\Gamma(q)$ belongs to $L^2(0, 1)$, and it is immediate from (2.14) that $\widehat{\psi}$ is locally H^2 on $(0, 1)$. Since $\theta \geq 1$, it follows that $\Gamma(q)$ is locally in H^1. Thus $Q - q$ is one degree smoother than q, meaning that Q, obtained by solving the regular problem, captures all discontinuities of q inside $(0, 1)$. Likewise if q is C^k or H^k then $q - Q$ is C^{k+1} or H^{k+1} locally.

It is also possible to seek the potential q as a solution of the operator equation (2.17). One can show that a convergent fixed point iteration scheme can be based on this equation, but there does not seem to be any advantage to this approach from a computational point of view.

2.3. The case $\ell = 1$

The transformation above for the $\ell = 2$ case changes the value of ℓ by 2, so by stringing such transformations together we can handle any even ℓ, see Section 2.5. For the case of odd ℓ we are in need of a way to handle the singular problem when $\ell = 1$. By modifying the earlier method we can make a transformation between the $\ell = 1$ and $\ell = 0$ cases, but a new complication then arises, which is that the boundary condition for the $\ell = 0$ problem at $x = 0$ becomes one of the unknowns.

With $\widehat{\lambda}$ and $\widehat{\rho}^+$ as before, the augmented spectral data $\{\mu_n, \sigma_n\}$ defined by (2.5), (2.6) have the correct properties for there to exist a unique $Q \in L^2(0, 1)$ and constant $h \in \mathbb{R}$ such that μ_n and σ_n are respectively eigenvalues and norming constants for

$$-u'' + Q(x)u = \lambda u \quad 0 < x < 1 \qquad u'(0) - hu(0) = u(1) = 0. \tag{2.18}$$

The norming constant in this case has the same definition as in (2.4) but the necessary and sufficient condition on this sequence becomes

$$\sigma_n = \frac{2}{((2n-1)\pi)^2}\left(1 + \frac{\beta_n}{n}\right) \qquad \sum_{n=1}^{\infty}\beta_n^2 < \infty \tag{2.19}$$

while the eigenvalue asymptotics is

$$\mu_n = \left(\left(n - \frac{1}{2}\right)\pi\right)^2 + C_0 + \alpha_n \qquad \sum_{n=1}^{\infty} \alpha_n^2 < \infty. \tag{2.20}$$

The relationship between q and Q becomes

$$q(x) = Q(x) - \frac{2}{x^2} - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\theta(x) \tag{2.21}$$

where θ is again defined by (2.9), (2.10). As in Section 2.1, one shows that $q \in L^2(0, 1)$.

An analytical example may be found as in the $\ell = 2$ case, namely if the spectral data is

$$\lambda_n = \left(\left(n + \frac{1}{2}\right)\pi\right)^2 \qquad \rho_n^+ = \frac{2}{((2n+1)\pi)^2} \tag{2.22}$$

then $h = 0$ and

$$q(x) = \frac{2\pi^2(2 + 2\cos\pi x + \pi x \sin\pi x)}{(\pi x + \sin\pi x)^2} - \frac{2}{x^2}. \tag{2.23}$$

2.4. Estimating the boundary condition

The new difficulty for the $\ell = 1$ case is the step of determining the constant h in the boundary condition. While unambiguous from a theoretical point of view, it does not seem that any of the constructive methods which have been developed for various versions of the regular inverse Sturm–Liouville problem confront this difficulty.

We consider therefore the regular Sturm–Liouville problem (2.18) with focus on the question of how to best estimate h from the data $\{\mu_n, \sigma_n\}$. Here $\{\mu_n\}$ are the eigenvalues of (2.18) and $\sigma_n = \int_0^1 \psi_n^2(x)\,\mathrm{d}x$ with ψ_n being the eigenfunction normalized at $x = 1$ as in (1.6). We also denote

$$\xi_n = \int_0^1 \phi_n^2(x)\,\mathrm{d}x \tag{2.24}$$

$$\zeta_n = \sqrt{\frac{\xi_n}{\sigma_n}} \tag{2.25}$$

where ϕ_n is the eigenfunction normalized by

$$\phi_n(0) = 1 \qquad \phi_n'(0) = h. \tag{2.26}$$

First we observe that

$$h = \sum_{n=1}^{\infty}\left[2 - \frac{1}{\xi_n}\right]. \tag{2.27}$$

This follows from standard formulas from the Gelfand–Levitan theory[3] (see for example [13,14]), specifically the property that $h = -F(0, 0)$ where

$$F(x, y) = \sum_{n=1}^{\infty}\left[\frac{1}{\xi_n}\cos\sqrt{\lambda_n}x\cos\sqrt{\lambda_n}y - 2\cos n\pi x\cos n\pi y\right]. \tag{2.28}$$

We also clearly have

$$\zeta_n = \frac{\phi_n}{\psi_n} = \frac{\phi_n'}{\psi_n'} = \frac{1}{\psi_n(0)} = \phi_n'(1) = \phi'(1, \mu_n) \tag{2.29}$$

where $\phi(x, \lambda)$ denotes the solution of the initial value problem

$$-u'' + Q(x)u = \lambda u \qquad \phi(0, \lambda) = 1 \qquad \phi'(0, \lambda) = h. \tag{2.30}$$

If we denote by $\Delta(\lambda) = \psi'(0, \lambda) - h\psi(0, \lambda)$ so that $\Delta(\mu_n) = 0$ for all n, then by a standard calculation we get

$$\int_0^1 \psi^2(x, \lambda) = \psi(0, \lambda)\dot{\Delta}(\lambda) \tag{2.31}$$

[3] Adapted to the case of a Dirichlet condition at one endpoint and a Robin condition at the other.

where the dot denotes derivative with respect to λ. In particular

$$\sigma_n = \frac{\dot{\Delta}(\lambda_n)}{\zeta_n} \tag{2.32}$$

so that

$$\xi_n = \sigma_n \zeta_n^2 = \frac{(\sigma_n \zeta_n)^2}{\sigma_n} = \frac{[\dot{\Delta}(\lambda_n)]^2}{\sigma_n}. \tag{2.33}$$

We have thus obtained

Lemma 2.1. *The boundary condition may be obtained from the spectral data by means of the absolutely convergent series*

$$h = \sum_{n=1}^{\infty} \left(2 - \frac{\sigma_n}{[\dot{\Delta}(\lambda_n)]^2} \right). \tag{2.34}$$

The absolute convergence of the series may be derived, for example, from (1.1.30) in [14] (after rescaling the interval to be [0, 1]) which implies that

$$2 - \frac{\sigma_n}{\dot{\Delta}(\lambda_n)^2} = 2 - \frac{1}{\xi_n} = \frac{a_n}{n} \qquad \sum_{n=1}^{\infty} a_n^2 < \infty. \tag{2.35}$$

2.5. Higher values of ℓ

The method of Section 2.1 may be used to transform an inverse spectral problem for any integer $\ell > 2$ to the corresponding problem when ℓ is replaced by $\ell - 2$. Thus any of these cases is reducible either to the $\ell = 1$ or $\ell = 2$ cases which have been treated in detail above. Here is a specific reconstruction algorithm:

Step 1. Choose numbers $\mu_1 < \mu_2 < \cdots \mu_\nu < \lambda_1$, and $\beta_1, \beta_2, \ldots, \beta_\nu > 0$, where $\nu = \frac{\ell}{2}$ if ℓ is even and $\nu = \frac{\ell+1}{2}$ if ℓ is odd.

Step 2. If ℓ is even find $Q \in L^2(0, 1)$ such that

$$\{\mu_1, \ldots, \mu_\nu\} \cup \{\lambda_n\}_{n=1}^{\infty}, \{\beta_1, \ldots, \beta_\nu\} \cup \{\rho_n^+\}_{n=1}^{\infty} \tag{2.36}$$

are the eigenvalues and norming constants of the regular Sturm–Liouville problem (2.1). If ℓ is odd find $Q \in L^2(0, 1)$ and $h \in \mathbb{R}$ such that (2.36) are the eigenvalues and norming constants of the regular Sturm–Liouville problem (2.18).

Step 3. If ℓ is even remove consecutively the ν eigenvalues $\mu_1, \ldots \mu_\nu$ from the spectrum by the procedure of Section 2.1 and its analogue in Appendix C for higher ℓ. If ℓ is odd remove μ_1 from the spectrum by the procedure of Section 2.3, and the remaining $\mu_2, \ldots, \mu_\nu$ by the procedure of Section 2.1 and Appendix C.

In all cases one will obtain $q \in L^2(0, 1)$ with the prescribed Dirichlet spectrum and norming constants for the given value of ℓ; we recall such a q is unique by Theorem 1.4.

3. Numerical methods

3.1. Description of the algorithm

In this section we describe in detail a computational method for the singular inverse spectral problem based on the discussions above, and give numerical examples. We begin again with the $\ell = 2$ case.

We assume that we are given a finite number of eigenvalues $\{\lambda_n\}_{n=1}^N$ and norming constants $\{\rho_n^+\}_{n=1}^N$ coming from some $q \in L^2(0, 1)$. An estimate for the mean value

$$\int_0^1 q(s)\, ds = \lim_{n \to \infty} (\lambda_n - ((n+1)\pi)^2) + 6 \tag{3.1}$$

may be immediately obtained from, e.g. $\lambda_N - ((N+1)\pi)^2 + 6$, or some extrapolation based on the last few λ_n's. Denote this estimate by $\bar{q}$.

For the augmented data (2.5), (2.6) we may choose any $\widehat{\lambda} < \lambda_1$ and $\widehat{\rho}^+ > 0$, but it is natural to choose them to be most consistent with the available information,

$$\widehat{\lambda} = \pi^2 + \bar{q} - 6 \qquad \widehat{\rho}^+ = \frac{1}{2\pi^2} \tag{3.2}$$

provided this choice does not contradict $\widehat{\lambda} < \lambda_1$. The computation of a discrete approximation to $Q(x)$, solution of the regular inverse Sturm–Liouville problem, may be carried out by the method of [15]—note that it is assumed there that the norming constant is given by $\|u_n\|_{L^2}^2/(u_n'(0))^2$, thus applying that method directly we obtain the reflected potential $Q(1-x)$. A brief review of this method is given in Appendix A.

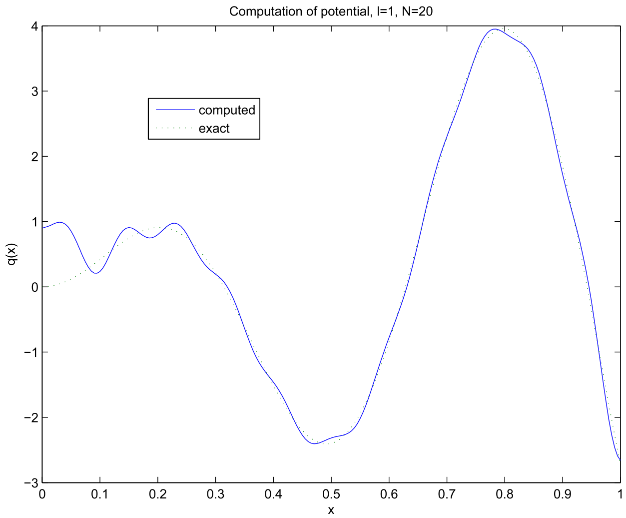

Fig. 1. Reconstruction of potential from spectral data, $\ell = 1, N = 20$.

The approximate solution $\widehat{\psi}$ of (2.10) may next be computed with the use of any convenient ODE solver, and then θ by some quadrature rule. We take care to compute these with high accuracy, especially in the vicinity of $x = 0$ in anticipation of the last step where equal singularities must cancel each other. We conclude by computing q from (2.8). Note that an equivalent expression for the second derivative of $\log\theta$ is

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\theta(x) = \frac{\widehat{\psi}(x)}{\theta^2(x)}\left(2\widehat{\psi}'(x)\theta(x) - \widehat{\psi}^3(x)\right). \tag{3.3}$$

In the step of computing $\widehat{\psi}$ the Eq. (2.10) is written as a first order system, thus both $\widehat{\psi}$ and $\widehat{\psi}'$ are returned in that solution, so no numerical differentiation needs to be done to evaluate the right hand side of (3.3).

For the $\ell = 1$ case we must begin by estimating the boundary parameter h from the given spectral data, using (2.34). We note that according to 1.1.28 of [14], we have the product formula for Δ in terms of its zeros (after rescaling to the interval $(0, 1)$),

$$\Delta(\lambda) = \prod_{n=1}^{\infty}\frac{\lambda_n - \lambda}{\lambda_{0n}} \tag{3.4}$$

where $\lambda_{0n} = ((n - \frac{1}{2})\pi)^2$. As a numerical matter, the evaluation of $\dot{\Delta}(\lambda_n)$ will need to be done carefully, using an equivalent formula such as

$$\dot{\Delta}(\lambda_n) = \frac{\cos\sqrt{\lambda_n}}{\lambda_n - \lambda_{0n}}\prod_{m\neq n}\frac{\lambda_m - \lambda_n}{\lambda_{0m} - \lambda_n} \tag{3.5}$$

which may be derived from (3.4) and the standard factorization

$$\cos z = \prod_{n=1}^{\infty}\left(1 - \frac{z^2}{\lambda_{0n}}\right). \tag{3.6}$$

Once the estimate for h is known, the numerical solution of the corresponding regular inverse problem for Q is obtained by a modification of the method of [15], see Appendix A. The remainder of the calculation proceeds as in the $\ell = 2$ case.

3.2. Numerical examples

We display numerical examples of the method just described for $\ell = 1$ and $\ell = 2$ in which $q(x) = 5x\sin 10x$. The eigenvalues of the singular problem are obtained with high accuracy from the MATLAB package MATSLISE [16]. Once the eigenvalues are known the eigenfunctions and subsequently the norming constants can be computed with a convenient ODE solver—the MATLAB command ODE45 was used in this case. In the examples $N = 20$ eigenvalues and norming constants were used, and the computation of q was done on a grid of 201 equally spaced points in $[0, 1]$. The results for $\ell = 1$ and $\ell = 2$ are shown in Figs. 1 and 2 respectively.

Comparison of the two figures shows a much greater tendency for oscillation of the computed solution in the $\ell = 1$ case, especially near the left endpoint, while for $\ell = 2$ the computed solution is smooth and more accurate over a large part of

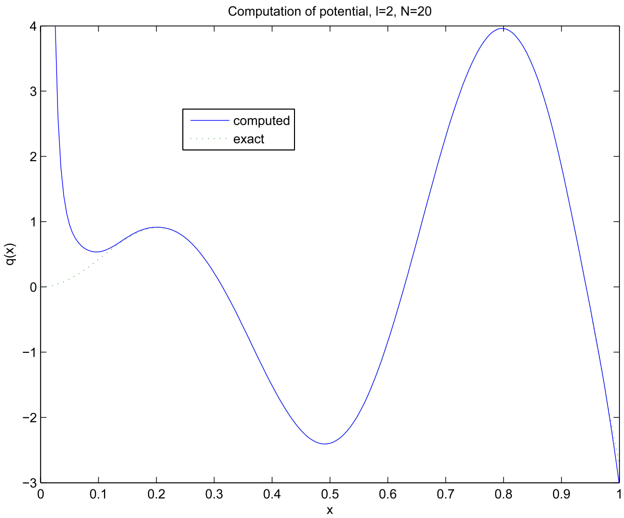

Fig. 2. Reconstruction of potential from spectral data, $\ell = 2$, $N = 20$.

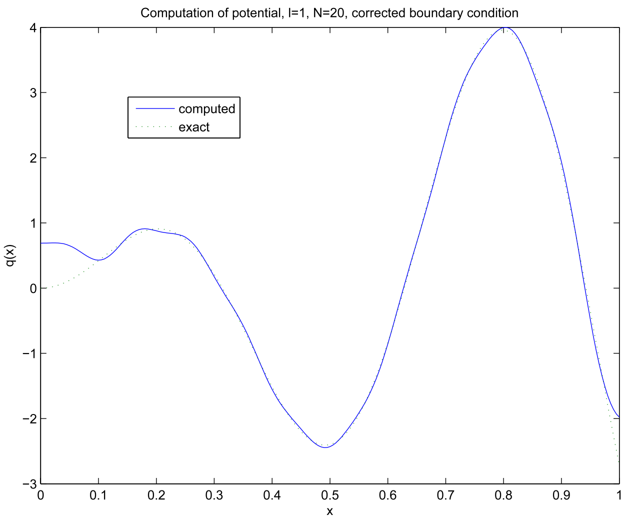

Fig. 3. Reconstruction of potential from spectral data, $\ell = 1$, $N = 20$ and correction to h.

the interval, but becomes completely inaccurate near $x = 0$. The excessive oscillation in the $\ell = 1$ case seems to be due to the computation of Q, and hence q, being very sensitive to the value of the boundary parameter h, and so indicates a failure to estimate this value well enough. In Fig. 3 a second reconstruction in the $\ell = 1$ case is shown, with the only difference being that a slightly different estimate of h is used, obtained by regarding Q as a function of h, and then minimizing the BV norm of Q in a neighborhood of the value of h found above. For the example displayed, it amounts to about a 1% change in the value of h, from $h \approx -.598$ to $h \approx -.593$. This estimation method will only make sense if there is reason to believe that q is sufficiently smooth so that significant oscillations in the computed solution can clearly be attributed to errors in the data.

The extreme loss of accuracy near $x = 0$ in the $\ell = 2$ case is due to the fact that $\theta = O(x^3)$ (see (3.3)) in this case, while it is only $O(x)$ when $\ell = 1$.

For a smooth potential such as in the above examples one expects that a much smaller value of N is sufficient for a very accurate reconstruction, at least in the regular $\ell = 0$ case. For $\ell = 2$ it seems similar, see Fig. 4 for the case $N = 4$. But in the case of $\ell = 1$ the reconstruction for $N = 4$ is not nearly as good, mainly due to the difficulty of estimating the boundary condition parameter h from so little data. In Fig. 5 we show the result for $N = 8$, and using a correction to h estimated as above.

Acknowledgement

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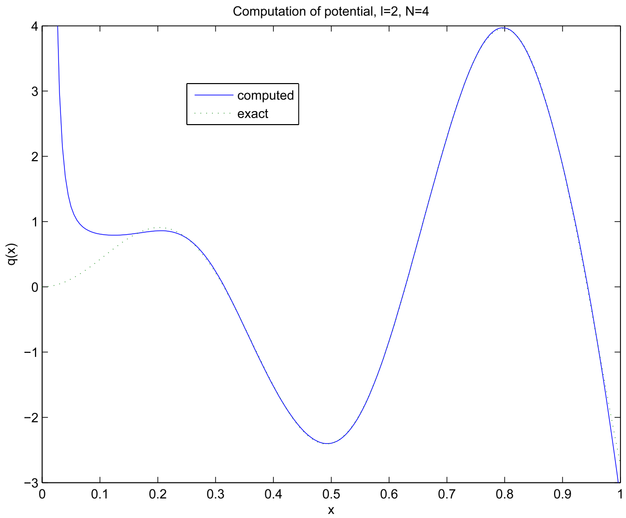

Fig. 4. Reconstruction of potential from spectral data, $\ell = 2$, $N = 4$.

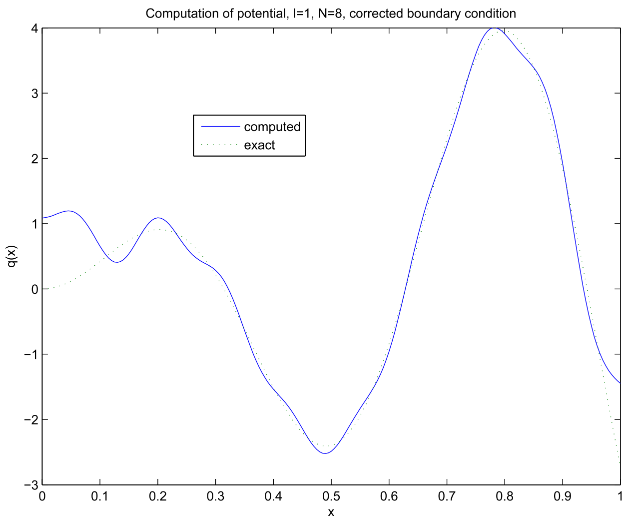

Fig. 5. Reconstruction of potential from spectral data, $\ell = 1$, $N = 8$ and correction to h.

Appendix A. Numerical method for the regular case

The numerical method from [15] for the regular inverse Sturm–Liouville problem may be used essentially without change in the $\ell = 2$ case, but when $\ell = 1$ the problem that must be solved does not quite match with any of those considered in [15]. Thus we briefly review the method and explain how it may be adapted to that case.

Consider the problem of recovering $V \in L^2(0, 1)$ from $\{\lambda_n, \rho_n\}$, where λ_n are eigenvalues of

$$y'' + (\lambda - V(x))y = 0 \quad 0 < x < 1 \tag{A.1}$$

$$y(0) = 0 \qquad y'(1) = Hy(1) \tag{A.2}$$

for $-\infty < H \leq \infty$, where as usual $H = \infty$ refers to the Dirichlet boundary condition $y(1) = 0$. The norming constants are

$$\rho_n = \int_0^1 \phi(x, \lambda_n)^2 \, dx \tag{A.3}$$

where ϕ is the solution of (A.1) satisfying $\phi(0, \lambda) = 0$, $\phi'(0, \lambda) = 1$. We encountered this problem in the $\ell = 2$ case with $H = \infty$ and $V(x) = Q(1 - x)$, and in the $\ell = 1$ case with $H = h$ for an unknown h, and again $V(x) = Q(1 - x)$.

We use the standard transformation formula

$$\phi(x, \lambda) = \frac{\sin\sqrt{\lambda}x}{\sqrt{\lambda}} + \int_0^x K(x, t)\frac{\sin\sqrt{\lambda}t}{\sqrt{\lambda}} \, dt \tag{A.4}$$

where the kernel K has certain properties. The general approach of [15] is to use the given spectral data to obtain the pair of functions $\{K_t(1,t), K_x(1,t)\}$, after which an iterative method may be used to find $V(x)$.

In the simpler $\ell = 2$ case, the identity $\phi(1,\lambda_n) = 0$ yields

$$\int_0^1 K_t(1,t)\cos\sqrt{\lambda_n}t\,\mathrm{d}t = -\sqrt{\lambda_n}\sin\sqrt{\lambda_n} - K(1,1)\cos\sqrt{\lambda_n} \tag{A.5}$$

and differentiating with respect to x we get

$$\int_0^1 K_x(1,t)\sin\sqrt{\lambda_n}t\,\mathrm{d}t = \sqrt{\lambda_n}\left(\kappa_n - \cos\sqrt{\lambda_n}\right) - K(1,1)\sin\sqrt{\lambda_n} \tag{A.6}$$

where $\kappa_n := \phi'(1,\lambda_n)$. By the discussion on 168–169 in [15]

$$\kappa_n = -\frac{\rho_n\sqrt{\lambda_n}(n^2\pi^2 - \lambda_n)}{\sin\sqrt{\lambda_n}}\prod_{m\neq n}\left(\frac{m^2\pi^2 - \lambda_n}{\lambda_m - \lambda_n}\right). \tag{A.7}$$

In addition,

$$K(1,1) = \frac{1}{2}\int_0^1 V(s)\,\mathrm{d}s = \frac{1}{2}\lim_{n\to\infty}(\lambda_n - n^2\pi^2) \tag{A.8}$$

so that the right hand sides of (A.5) and (A.6) depend only on the given spectral data. It may then be shown that $K_t(1,t)$ and $K_x(1,t)$ are uniquely determined, and thus so is V. In practice, we use (A.8) to estimate the value of $\overline{V} = \lim_{n\to\infty}\lambda_n - n^2\pi^2$, then replace λ_n by $\lambda_n - \overline{V}$ and $V(x)$ by $V(x) - \overline{V}$, to achieve the slightly simpler situation that $K(1,1) = 0$.

In the $\ell = 1$ case, when H is finite, we set $\kappa_n = \phi(1,\lambda_n)$ and may then compute that

$$\int_0^1 K_t(1,t)\cos\sqrt{\lambda_n}t\,\mathrm{d}t = \lambda_n\kappa_n - \sqrt{\lambda_n}\sin\sqrt{\lambda_n} + K(1,1)\cos\sqrt{\lambda_n} \tag{A.9}$$

$$\int_0^1 K_x(1,t)\sin\sqrt{\lambda_n}t\,\mathrm{d}t = -H\sqrt{\lambda_n}\kappa_n - \sqrt{\lambda_n}\cos\sqrt{\lambda_n} - K(1,1)\sin\sqrt{\lambda_n}. \tag{A.10}$$

By earlier discussion we have

$$\kappa_n = \frac{\rho_n}{\dot{\Delta}(\lambda_n)} \tag{A.11}$$

with $\dot{\Delta}(\lambda_n)$ given by (3.5). The eigenvalue asymptotics are

$$\lambda_n \approx \left(\left(n - \frac{1}{2}\right)\pi\right)^2 + \int_0^1 V(s)\,\mathrm{d}s + 2H. \tag{A.12}$$

The value of H is in principle obtained from Lemma 2.1, that is

$$H = \sum_{n=1}^{\infty}\left(2 - \frac{\rho_n}{[\dot{\Delta}(\lambda_n)]^2}\right) \tag{A.13}$$

after which we get $\int_0^1 V(s)\,\mathrm{d}s$, or equivalently the value of $K(1,1)$ from (A.12).

Appendix B. Hardy operators

In this section we briefly discuss some properties of mappings of Hardy type.

Lemma B.1. *Assume $n \in \mathbb{Z}_+$ and $\alpha > n + \frac{1}{2}$; then the operator*

$$T_\alpha : f \mapsto \frac{1}{x^\alpha}\int_0^x t^{\alpha-1}f(t)\,\mathrm{d}t \tag{B.1}$$

is continuous in the Sobolev space $H^n(0,1)$.

Proof. Continuity of T_α in $H^n(0,1)$ is justified by induction in n. For $n = 0$, T_α is a continuous linear transformation of $L^2(0,1)$ by [17, Sect. 9.9].

Assume the claim is already established for all $n < k$; we shall now prove that it also holds for $n = k$. Let therefore $\alpha > k + \frac{1}{2}$ and $f \in H^k(0,1)$; writing $T_\alpha f$ as

$$T_\alpha f(x) = \frac{f(x)}{\alpha} - \frac{1}{\alpha x^\alpha}\int_0^x t^\alpha f'(t)\,\mathrm{d}t \tag{B.2}$$

we see that it suffices to show that the mapping

$$f \mapsto g(x) := -\frac{1}{\alpha x^\alpha}\int_0^x t^\alpha f'(t)\,\mathrm{d}t \tag{B.3}$$

is continuous in $H^k(0,1)$. The relation

$$g'(x) = \frac{1}{x^{\alpha+1}}\int_0^x t^\alpha f'(t)\,\mathrm{d}t - \frac{f'(x)}{\alpha} \tag{B.4}$$

and the induction assumption show that $g' \in H^{k-1}(0,1)$ and that the map $f' \mapsto g'$ is continuous in $H^{k-1}(0,1)$. Therefore g belongs to $H^k(0,1)$ and depends continuously therein on $f \in H^k(0,1)$. This justifies the induction step and completes the proof. □

Corollary B.2. *Assume that $f \in H^2(0,1)$ and $f(0) \neq 0$. Then the function*

$$g(x) := \frac{1}{x^3}\int_0^x t^2 f^2(t)\,\mathrm{d}t \tag{B.5}$$

belongs to $H^2(0,1)$ and is positive on $[0,1]$.

Proof. In view of the above lemma, g belongs to $H^2(0,1)$ and thus is continuous on $[0,1]$ by the Sobolev imbedding theorem. Clearly, $g(x) > 0$ for all $x > 0$. By L'Hospital's rule, we get that $g(0) = f^2(0)/3 > 0$, so that g is positive on $[0,1]$. □

Lemma B.3. *Assume that $a \in L^2(0,1)$ and let ϕ be a non-trivial solution of the equation*

$$\phi'' = a\phi \tag{B.6}$$

subject to the initial condition $\phi(0) = 0$. Then $\phi(x)/x \in H^2(0,1)$.

Proof. Regularity theorem for solutions of Sturm–Liouville equations implies that $\phi \in H^2(0,1)$; thus

$$\frac{\phi(x)}{x} = \frac{1}{x}\int_0^x \phi'(t)\,\mathrm{d}t \tag{B.7}$$

belongs to $L^2(0,1)$ by Lemma B.1. Since $\lim_{x\to 0}\phi(x)/x = \phi'(0)$, the function $\phi(x)/x$ is continuous on $[0,1]$, whence

$$\psi(x) := \frac{\phi''(x)}{x} = a(x)\frac{\phi(x)}{x} \in L^2(0,1). \tag{B.8}$$

Next we find that

$$\left(\frac{\phi(x)}{x}\right)' = \frac{\phi'(x)}{x} - \frac{\phi(x)}{x^2} = \frac{1}{x^2}\int_0^x t\phi''(t)\,\mathrm{d}t \tag{B.9}$$

$$= \frac{1}{x^2}\int_0^x t^2\psi(t)\,\mathrm{d}t =: \chi(x). \tag{B.10}$$

The function χ is clearly absolutely continuous on $(0,1]$ and the estimate $|\chi(x)| \le \int_0^x |\psi(t)|\,\mathrm{d}t$ shows that $\chi(x) \to 0$ as $x \to 0$, so that $\chi \in C[0,1]$. Finally, we have

$$\chi'(x) = -\frac{2}{x^3}\int_0^x t^2\psi(t)\,\mathrm{d}t + \psi(x) \in L^2(0,1) \tag{B.11}$$

by Lemma B.1 and (B.8), so that $\chi \in H^1(0,1)$ and $\phi(x)/x \in H^2(0,1)$. □

Lemma B.4. *The mapping Γ of (2.16) preserves $L^2(0,1)$.*

Proof. Slightly adapting the arguments of [3] one can show that the solution $\widehat{\psi}$ of (2.14) has the form $\widehat{\psi}(x) = x^{-2}\omega(x)$ for some $\omega \in H^2(0,1)$ that is positive on $[0,1)$. Reasoning analogous to that used in the proof of Lemma B.1 (cf. also Lemma A.3 of [3]) shows that the mapping

$$f \mapsto x^3\int_x^1 \frac{f(t)}{t^4}\,\mathrm{d}t \tag{B.12}$$

is continuous in $H^2(0,1)$, so that the function $\theta(x) - 1$ has the form $x^{-3}\chi(x)$ for some nonnegative $\chi \in H^2(0,1)$ with $\chi(0) = \omega^2(0)/3 > 0$. Therefore

$$\theta(x) = x^{-3}\chi_1(x) \tag{B.13}$$

with $\chi_1(x) = x^3 + \chi(x) \in H^2(0, 1)$. Since χ_1 is positive on $[0, 1]$, we find that

$$\Gamma(q) = -2\frac{d^2}{dx^2}\log\chi_1 \in L^2(0, 1) \tag{B.14}$$

as claimed. □

Appendix C. Double commutation transformation

In this appendix, we give a brief account of the double commutation method that allows one to insert or remove eigenvalues of a Bessel operator while leaving all the norming constants unchanged. For details, see [2], the paper [12] which discusses the transformation in a more general context and e.g. [3] which investigates the effect of such transformations on spectra of the Bessel operators in factorised form on a finite interval.

C.1. Transformation

Assume that $f \in L^2_{loc}(0, 1]$ and $\alpha \in \mathbb{R} \setminus \{0\}$ are such that $\alpha\int_x^1 |f(s)|^2\,ds > -1$ for all $x \in (0, 1]$. We denote by $U = U(f, \alpha)$ an operator in $L^2_{loc}(0, 1]$ given by (cf. [12])

$$(Ug)(x) := g(x) - \frac{\alpha f(x)}{1 + \alpha\int_x^1 |f(s)|^2\,ds}\int_x^1 g(s)\overline{f(s)}\,ds \tag{C.1}$$

in particular,

$$(Uf)(x) = \frac{f(x)}{1 + \alpha\int_x^1 |f(s)|^2\,ds}. \tag{C.2}$$

The inverse transformation U^{-1} is easily seen to be [12]

$$(U^{-1}g)(x) = g(x) + \alpha f(x)\int_x^1 g(s)\overline{(Uf)(s)}\,ds. \tag{C.3}$$

Direct calculations (involving integration by parts and simple algebra) give

$$\int_x^1 |(Ug)(s)|^2\,ds = \int_x^1 |g(s)|^2\,ds - \alpha\frac{\left|\int_x^1 g(s)\overline{f(s)}\,ds\right|^2}{1 + \alpha\int_x^1 |f(s)|^2\,ds} \tag{C.4}$$

in particular,

$$\int_x^1 |(Uf)(s)|^2\,ds = \frac{1}{\alpha}\left[1 - \left(1 + \alpha\int_x^1 |f(s)|^2\,ds\right)^{-1}\right] \tag{C.5}$$

so that $Uf \in L^2(0, 1)$ if and only if either $f \notin L^2(0, 1)$ or $f \in L^2(0, 1)$ and $1 + \alpha\|f\|^2 > 0$.

Combining the above properties of the mapping U, we conclude the following (see [12, Lemma 2.1]).

Proposition C.1. *The operator U performs a unitary equivalence of $L^2(0, 1) \ominus f$ and $L^2(0, 1) \ominus Uf$; here $L^2(0, 1) \ominus f = L^2(0, 1)$ if f is not in $L^2(0, 1)$, and similarly for $L^2(0, 1) \ominus Uf$.*

C.2. Differential equations

Let now $q \in L^2_{loc}(0, 1]$ and denote by $y(\cdot, \lambda)$ a solution of the equation

$$-y'' + q_0 y = \lambda y \tag{C.6}$$

subject to the terminal conditions $y(1) = 0$ and $y'(1) = 1$. We next choose $\lambda_* \in \mathbb{R} \setminus \{0\}$ and $\alpha_* \in \mathbb{R} \setminus \{0\}$ so that the function

$$w(x) := 1 + \alpha_*\int_x^1 |y(t, \lambda_*)|^2\,dt \tag{C.7}$$

does not vanish on $(0, 1]$ and consider the transformation

$$U_* := U\big(y(\cdot, \lambda_*), \alpha_*\big). \tag{C.8}$$

We set $q_*(x) := q_0(x) - 2\frac{d^2}{dx^2}\log w(x)$ and $u(\cdot, \lambda) := Uy(\cdot, \lambda)$ for $\lambda \in \mathbb{C}$; then the following holds true (cf. [3,12]).

Proposition C.2. *The function $u(\cdot, \lambda)$ satisfies the equation*

$$-u'' + q_* u = \lambda u \tag{C.9}$$

and the terminal conditions $u(1) = 0$ and $u'(1) = 1$.

Using the above two propositions, we can justify the spectral effect of the transformation U on Bessel operators used in Section 2. Namely, let $q_0(x) = Q(x) + \ell(\ell+1)/x^2$ with $\ell \ge 0$ and let $\lambda_1 < \lambda_2 < \cdots$ be all the eigenvalues and $\rho_1^+, \rho_2^+, \ldots$ the norming constants of the corresponding Bessel operator (for $\ell = 0$ we need an extra Dirichlet or Robin boundary condition at $x = 0$).

C.3. Removing an eigenvalue

Take $\lambda_* := \lambda_k$ for some $k \in \mathbb{N}$ and $\alpha_* := -1/\rho_k^+$. Then the above transformation U_* maps the functions $y(\cdot, \lambda_n)$ into functions $u(\cdot, \lambda_n)$ that for $n \ne k$ belong to $L^2(0, 1)$, are pairwise-orthogonal there, satisfy the Dirichlet condition $u(1) = 0$ and solve Eqs. (C.9) with respective λ and q_*. Isometric properties of U_* imply that $u(\cdot, \lambda_k)$ does not belong to $L^2(0, 1)$ while $\|u(\cdot, \lambda_n)\| = \|y(\cdot, \lambda_n)\|$ for $n \ne k$.

Moreover, the reasoning similar to that used in Appendix B shows that

$$w(x) = 1 - \frac{1}{\rho_k^+} \int_x^1 y^2(s, \lambda_k)\, \mathrm{d}s \tag{C.10}$$

$$= \frac{1}{\rho_k^+} \int_0^x y^2(s, \lambda_k)\, \mathrm{d}s = x^{2\ell+3} \widehat{w}(x) \tag{C.11}$$

for some $\widehat{w} \in H^2(0, 1)$ that is positive on $[0, 1]$ provided $\ell > 0$ or $\ell = 0$ but the boundary condition at $x = 0$ is the Dirichlet one; in particular if $q(x) = q_*(x) - (\ell+2)(\ell+3)/x^2$ then

$$q(x) + \frac{(\ell+2)(\ell+3)}{x^2} = Q(x) + \frac{\ell(\ell+1)}{x^2} - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2} \log w(x) \tag{C.12}$$

or

$$q(x) = Q(x) - \frac{4\ell+6}{x^2} - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2} \log w(x). \tag{C.13}$$

For $\ell = 0$ and $k = 1$, this is the formula (2.8), since $w(x)$ here is the same as θ in that formula. If $\ell = 0$ and the boundary condition at $x = 0$ is of Robin type, then one gets that $w(x) = x\widehat{w}(x)$ for some $\widehat{w} \in H^2(0, 1)$ which is positive on $[0, 1]$ from which (2.21) follows in a similar manner. It thus follows that the Bessel operator (1.1) with potential q and ℓ changed to $\ell + 2$ has eigenvalues λ_n, $n \ne k$, and the corresponding norming constants are ρ_n^+.

C.4. Adding an eigenvalue

Assume $\ell \ge 1$ and take $\lambda_* := \widehat{\lambda} \in (0, \lambda_1)$ and $\alpha_* := 1/\widehat{\rho} > 0$. Then the above transformation U_* maps the functions $y(\cdot, \widehat{\lambda})$ and $y(\cdot, \lambda_n)$ into functions $u(\cdot, \widehat{\lambda})$ and $u(\cdot, \lambda_n)$ that are pairwise orthogonal in $L^2(0, 1)$, satisfy the Dirichlet condition $u(1) = 0$ and solve Eqs. (C.9) with respective λ and q_*. Isometric properties of U_* show that $\|u(\cdot, \lambda_n)\|^2 = \rho_n^+$, while (C.5) yields $\|u(\cdot, \widehat{\lambda})\|^2 = \widehat{\rho}$.

If $\ell \ge 3$, then using $q_0(x) = q(x) + \ell(\ell+1)/x^2$ and $q_*(x) = Q(x) + (\ell-2)(\ell-1)/x^2$ we get

$$Q(x) = q(x) + \frac{4\ell-2}{x^2} - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2} \log w(x). \tag{C.14}$$

The same relation is valid when $\ell = 2$; then in addition it can be shown that all the functions $u(\cdot, \widehat{\lambda})$ and $u(\cdot, \lambda_n)$ vanish at $x = 0$, which implies (2.17). Finally for $\ell = 1$ one similarly proves that these functions satisfy a Robin-type condition at $x = 0$; see details in [3].

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